

**Nicholas W. Winter**

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**Education:**

California Institute of Technology, Pasadena, CA, attended from September 1965 to November 1969, PhD, June 1970.

Northern Illinois University, Dekalb, IL, attended from September 1962 to June 1965, B.S. (with Highest Honors), June 1965.

**Work History:**

Lawrence Livermore National Laboratory, Livermore, CA, Physicist, (1976–present).

California State University East Bay, Hayward, CA, Department of Chemistry and Biochemistry(1996–2001).

Aerospace Corporation, El Segundo, CA (1973–1976)

Associate Research Fellow, Applied Physics, California Institute of Technology, Pasadena, CA (1971–1975)

NRC Fellow, Jet Propulsion Laboratory, Pasadena, CA (1971–1973)

Postdoctoral Fellow, Battelle Memorial Institute, Columbus, OH (1969–1971)

**Graduate Students:**

Thomas. B. Stewart, *Influence of Initial Vibrational Energy on the BrH + I → Br + HI Exchange Reaction*, M.S., Department of Chemistry, UCLA 1978.

John Deisz, *Spin-Orbit Interaction in the excited States of CF<sub>3</sub>I*, M.S., Department of Applied Science, UCD 1987.

Barry A. Dahling, *High Pressure Studies of Chromium and Vanadium Doped Crystals*, M.S., Department of Applied Science, UCD 1990.

Dave K. Temple, *Ab Initio Cluster Study of Crystalline NaF*, Ph.D., Department of Applied Science, UCD 1992.

Tim Onasch, *NO adsorption on CuO*, SERS Student, 1993.

Mary A. Lee, *Theoretical Studies of Mineral Dissolution and Ligand Exchange*, Ph.D., Department of Chemistry, UCD 1996.

**Teaching:**

*Introduction to Computational Methods in Biochemistry*, Winter Quarter 1996  
*Advanced Inorganic Chemistry*, Fall & Winter Quarters 1997-1998  
*Molecular Spectroscopy*, Winter Quarter 1999  
*Structure-Activity and Structure-Property Relationships*, Winter Quarter 2000  
*Reaction Mechanisms in Organic Chemistry*, Fall Quarter 2000  
*Solids and Surfaces: A Chemist's View of Bonding in Extended Structures*, Winter Quarter 2001  
*Advanced Computational Methods for Macromolecules*, Spring Quarter 2001

**Awards and Honors:**

Fellow of Sigma Pi Sigma Physics Honor Society  
Fellow of Sigma Zeta Honor Society  
Chemical and Engineering News Merit Award

**Membership:**

American Physical Society  
American Chemical Society  
National Research Council, High Energy Density Materials Panel, (1985–1988).

**Publications:**Refereed Journal Articles:

F. H. Ree, N. W. Winter, J. N. Glosli, J. A. Viecelli, “Kinetics and thermodynamic behavior of carbon clusters under high pressure and high temperature”, *Physica B*, **265**, 223-229, (1999).

F. H. Ree, J. Glosli, and N. Winter, “Equilibrium and Nonequilibrium Properties of Bulk and Nanosize Clusters of Carbon”, *Rev. High Pressure Sci. Techn.*, **7**, 900, (1998).

N. W. Winter and F. H. Ree, “Carbon particle phase stability as a function of size”, *J. Comp.-Aided Mater.*, **5**, 279-294, (1998).

S. Parkin, G. A. Marsch, H. Hope, E. Whitney, N. W. Winter, M.E. Colvin, J. S. Felton, K. W. Turteltaub, “Comparison of crystal structure and theory for 2-amino-1-methyl-6-phenylimidazo[4,5-b]pyridine”, *Chem. Res. Toxicol.*, **9**, 574-579, (1996).

R. Vikse, F.T. Hatch, N.W. Winter, M.G. Knize, S. Grivas and J.S. Felton, “Structure-Mutagenicity Relationships of 4 Amino-Imidazonaphthyridines and Imidazoquinolines”, *Environ. Mol. Mutagen.*, **26**, 79-85, (1995).

- M. Ross, L. Yang, B. Dahling, and N. Winter, “The Insulator-Metal Transition in Expanded Cesium”, *Z. Phys. Chem.*, **184**, 65-72, (1994).
- M. J. Durst, C. E. Violet, N. W. Winter, Z. Mei, “Curve-Fitting Complex Mossbauer Spectra; Application to HoBa<sub>2</sub>(Cu0.95Fe0.05)3O<sub>7.02</sub>”, *Nucl. Instrum. Meth. B*, **93**, 521-529, (1994).
- M. A. Lee, N. W. Winter, and W. H. Casey, “Investigation of the Ligand-Exchange Reaction for the Aqueous Be<sup>2+</sup> Ion”, *J. Phys. Chem.*, **98**, 8641-8647, (1994).
- N. W. Winter, C.I. Merzbacher, C.E. Violet, “The Nuclear-Quadrupole Interaction in High-Temperature Superconductors”, *Appl. Spectrosc. Rev.*, **28**, 123-164, (1993).
- C. E. Violet, R. G. Bedford, N. W. Winter, G. S. Smith, Z. Mei, M. J. Durst, and J. K. Wu, “Fe<sup>57</sup> Mossbauer Spectrometry and Thermogravimetry of the High-Tc Superconductor HoBa<sub>2</sub>(Cu0.95Fe0.05)3O<sub>7.02</sub>”, *Physica C*, **207**, 347-358, (1993).
- R. M. Pitzer and N. W. Winter, “Spin-Orbit (Core) and Core Potential Integrals”, *Int. J. Quantum Chem.*, **40**, 773-780, (1991).
- R. B. Ross, C. W. Kern, R. M. Pitzer, W. C. Ermler, and N. W. Winter, “Ab Initio Properties of Electronic States of Be<sup>69</sup>”, *J. Phys. Chem.*, **94**, 7771-7774, (1990).
- N. W. Winter, M. Ross, and R. M. Pitzer, “Calculation of the Pressure Shifts of the Quartet States of Ruby”, *J. Phys. Chem.*, **94**, 1172-1174, (1990).
- N. W. Winter and C. E. Violet, “Calculation of the Nuclear Quadrupole Resonance Spectra of YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7-x</sub>”, *Physica C*, **162**, 261-262, (1989).
- C. E. Violet, R. G. Bedford, P. A. Hahn, N. W. Winter, and Z. Mei, “Local Oxygen Configurations Relative to Fe-Probe Ions in HoBa<sub>2</sub>(Cu0.95Fe0.05)3O<sub>7-x</sub>”, *Physica C*, **162**, 1291-1292, (1989).
- N. W. Winter and R. M. Pitzer, “Configuration-Interaction Calculation of the Electronic-Spectra of MgF<sub>2</sub>:V<sup>+2</sup>”, *J. Chem. Phys.*, **89**, 446-451, (1988).
- W. C. Ermler, R. B. Ross, C. W. Kern, R. M. Pitzer, and N. W. Winter, “Selected Properties of Be Clusters in Ab Initio Model Approximations”, *J. Phys. Chem.*, **92**, 3042-3046, (1988).
- R. M. Pitzer and N. W. Winter, “Electronic-Structure Methods for Heavy-Atom Molecules”, *J. Phys. Chem.*, **92**, 3061-3063, (1988).
- N. W. Winter, R. M. Pitzer and D. K. Temple, “Hartree-Fock Calculation of the Electronic Structure of a Cu<sup>+</sup> Impurity in NaCl”, *J. Chem. Phys.*, **87**, 2945-2953, (1987).
- N. W. Winter, R. M. Pitzer and D. K. Temple, “Theoretical Study of a Cu<sup>+</sup> Ion Impurity in a NaF Host”, *J. Chem. Phys.*, **86**, 3549-3556, (1987).

- N. W. Winter and D. L. Huestis, "Theoretical Description of the Low-Lying Excited States of CuCl", *Chem. Phys. Lett.*, **133**, 311-316, (1987).
- W. C. Ermler, C. W. Kern, R. M. Pitzer, and N. W. Winter, "Ab Initio Calculations on Electronic States of Be-13", *J. Chem. Phys.*, **84**, 3937-3943, (1986).
- J. H. Yates, W. C. Ermler, N. W. Winter, P. A. Christiansen, Y. S. Lee, and K. S. Pitzer, "Ab Initio Potential-Energy Curves for the Low-Lying Electronic States of the Argon Excimer", *J. Chem. Phys.*, **79**, 6145-6149, (1983).
- W. L. Morgan, N. W. Winter, K. C. Kulander, "Vibrational relaxation and laser extraction in rare gas halide excimers", *J. Appl. Phys.*, **54**, 4275-4279, (1983).
- P. A. Christiansen, K. S. Pitzer, Y. S. Lee, J. H. Yates, W. C. Ermler and N. W. Winter, "Improved ab initio effective potentials for Ar, Kr, and Xe with applications to their homonuclear dimers", *J. Chem. Phys.*, **75**, 5410-5415, (1981).
- M. R. Flannery, K. J. McCann, and N. W. Winter, "Cross sections for electron impact ionization of metastable rare-gas excimers (He $2^*$ , Kr $2^*$ , Xe $2^*$ )", *J. Phys. B-At. Mol. Opt.*, **14**, 3789-3796, (1981).
- F. H. Ree and N. W. Winter, "Ab initio and Gordon-Kim intermolecular potentials for two nitrogen molecules", *J. Chem. Phys.*, **73**, 322-336, (1980).
- W. C. Ermler, Y. S. Lee, K. S. Pitzer, and N. W. Winter, "Ab initio Effective Core Potentials Including Relativistic Effects. II. Potential Energy Curves for Xe $2$ , Xe $2^+$ , and Xe $2^{*+}$ ", *J. Chem. Phys.*, **69**, 976-983, (1978).
- C. F. Bender and N. W. Winter, "Theoretical Absorption Spectra of ArKr+", *Appl. Phys. Lett.*, **33**, 29-31, (1978).
- T. N. Rescigno, A. U. Hazi, and N. Winter, "Comments on the existence of low-energy d-wave resonances in electron-fluorine atom scattering", *Phys. Rev. A*, **16**, 2488-2490, (1977).
- N. W. Winter, C. F. Bender and T. N. Rescigno, "Potential energy curves and predicted fluorescence for neon fluoride", *J. Chem. Phys.*, **67**, 3122-3125, (1977).
- W. R. Wadt and N. W. Winter, "Accurate Characterization of the Transition State Geometry of the HF+H  $\rightarrow$  H+FH Reaction", *J. Chem. Phys.*, **67**, 3068-3073, (1977).
- Johnson, B R and Winter, N W, "Classical trajectory study of the effect of vibrational energy on the reaction of molecular hydrogen with atomic oxygen", *J. Chem. Phys.*, **66**, 4116-4120, (1977).
- N. W. Winter, W. A. Goddard, and F. W. Bobrowicz, "Configuration interaction studies of the excited states of water", *J. Chem. Phys.*, **62**, 4325-4331, (1975).
- N. W. Winter, "Theoretical assignments of the electronic states of nitrous oxide", *Chem.*

*Phys. Lett.*, **33**, 300-304, (1975).

N. W. Winter and W. A. Goddard, "Theoretical Description of the 2A" and 2A' states of the Peroxyformal Radical", *Chem. Phys. Lett.*, **33**, 25-29, (1975).

N. W. Winter, C. F. Bender and W. A. Goddard, "Theoretical assignments of the low-lying electronic states of carbon dioxide", *Chem. Phys. Lett.*, **20**, 489-492, (1973).

N. Winter, W. C. Ermler and R. M. Pitzer, "An algorithm for the use of symmetry in molecular self consistent field calculations", *Chem. Phys. Lett.* 19, 179 (1973)

N. W. Winter, "Electron correlation in the hydride ion", *J. Chem. Phys.* 56, 2267 (1972).

N. W. Winter and T. H. Dunning, "The barrier to internal rotation in hydrogen peroxide", *Chem. Phys. Lett.* 11, 194 (1971)

N. W. Winter and T. H. Dunning, "Accelerating the convergence of matrix Hartree Fock calculations", *Chem. Phys. Lett.* 8, 169 (1971)

N. W. Winter and V. McCoy, "Numerical solution of the (1s1s) and (1s2s) hydrogenic pair equations", *Phys. Rev. A2*, 2219 (1971)

N. W. Winter, A. Lafferriere, and V. McCoy, "Solution of the Hartree Fock first-order equation for the helium atom", *Chem. Phys. Lett.* 6, 175 1970)

N. W. Winter, A. Lafferriere, and V. McCoy, "Numerical solution of the two-electron Schrodinger equation", *Phys. Rev. A2*, 49 (1970)

T. H. Dunning and N. W. Winter, "Formaldehyde molecule in a Gaussian basis. Electron density plots", *J. Chem. Phys.* 55, 3360 (1971)

T. H. Dunning, N. W. Winter, and V. McCoy, "Formaldehyde molecule in a Gaussian basis. One-electron properties", *J. Chem. Phys.* 49, 4128 (1968)

N. W. Winter, T. H. Dunning and J. Letcher, "Formaldehyde molecule in a Gaussian basis. A self consistent field calculation", *J. Chem. Phys.* 49, 1871 (1968)

N. W. Winter and V. McCoy, "Numerical one-center calculation of the ns- $\sigma$  Rydberg series of  $H_2^+$ ", *J. Chem. Phys.* 49, 478 (1968)

N. W. Winter and V. McCoy, "Numerical solution of quantum mechanical pair equations", *J. Chem. Phys.* 48, 5514 (1968)

N. W. Winter, D. Diestler and V. McCoy, "Numerical solution of the S-limit Schrodinger equation", *J. Chem. Phys.* 48, 1879 (1968)

W. A. Yeranos and N. W. Winter, "Corrections to The quantum-mechanical calculation of one-electron properties. II. One and two center integrals", *A. Naturforsch.* 20a, 1217 (1965)

W. A. Yeranos and N. W. Winter, “Suggested semiempirical molecular orbital schemes for xenon tetroxide”, Bull. Soc. Chim. Belges, 75, 116 (1965)

Lawrence Livermore National Laboratory Reports:

John E. Reaugh, Thomas A. Reitter, and Nicholas W. Winter, “Grain-scale Dynamics and Burn Rates in Explosives Munitions Technology Development Program FY2005 Progress Report”, UCRL-TR-220232 (2006).

J. F. Holzrichter, G. L. Struble, A. K. McMahan, E. R. Mapoles, M. J. Fluss, E. N. Kaufmann, N. W. Winter, L. J. Summers, R. W. Moir, D. B. Tuckerman, H. D. Shay, D. H. Darlin& and G. R. Neil, “Applications of high temperature superconductors”, UCRL-53855 (1988).

Pitzer, R M and Winter, N M, “Relativistic Calculations On Polyatomic Systems”, UCRL-UCRL-93231 (1985).

N. W. Winter and T. N. Rescigno, “Theoretical Calculation Of The Bound-free Emission Spectra Of KrF”, UCRL-UCRL- 81623 (1978).

C. Bender, A. Hazi, A. Orel, T. Rescigno and N. Winter, “Theoretical Studies Involving Candidate Group Via Laser Systems”, UCRL-UCRL-80165 (1978).

Books:

N. W. Winter, D. K. Temple, V. Luana, and R. M. Pitzer, in *Advances in Molecular Electronic Structure Theory*, Vol. 2, editors: T.H. Dunning, (JAI Press Inc., , 1993), “Calculation of the Electronic Structure of Transition Metal Impurities in Ionic Crystals”, 61-109.

T.N. Rescigno and N.W. Winter, in *Electronic Transition Lasers II*, editors: L.E. Wilson, S.N. Suchard, and J.I. Steinfeld, (The MIT Press, Cambridge, MA, 1977), “Theoretical Modeling Of The KrF Fluorescence Spectrum”.

Published Conference Proceedings:

F. H. Ree, N. W. Winter, J. N. Glosli, and J. A. Viecelli, “High-Pressure, High-Temperature Behavior of Carbon in Chemically Reactive Environment”, AIRAPT 17, International Conference on High Pressure Science and Technology (Honolulu, HI, July 1999), *Science and Technology of High-Pressure Research*, M. H. Manghnani, W. J. Nellis, M. F. Nicol, eds. *Proc. Int. Conf.on High Pressure Science and Technology AIRAPT-17 (2000)*.

F. H. Ree, G. Galli, J. N. Glosli, F. Gygi, E. Schwegler, J. A. Viecelli, N. W. Winter, “Dynamic and Thermodynamic Behavior of Carboneous and Hydrogen-Bonding Materials”, Symposium on Shock Waves, Japan 2000 (Tokyo, Japan, March 2000), *Proceedings of the Symposium on Shock Waves, Japan 2000 (March 16-18)*.

F.H. Ree, N.W. Winter, J.N. Glosli, "Kinetics and thermodynamic behavior of carbon clusters under high pressure and high temperature", 36th European High Pressure Research Group Meeting on Molecular and Low Dimensional Systems under Pressure (Catalina, Italy, September 1998).

N. W. Winter and F. H Ree, "Stability of the Graphite and Diamond Phases of Finite Carbon Clusters", 11th International Detonation Symposium (Snowmass, CO, August 1998), *Proceeding of the 11th Int. Symposium on Detonation, ed. by J. Short, , pp 468* (1998).

N. W. Winter and R. M. Pitzer, "Theoretical Methods for the Study of Transition Metals in Crystals", Conference on Tunable Solid State Lasers (La Jolla, CA, June 1984), *Proceedings of the Conference on Tunable Solid State Lasers, ed. P. Hammerling (Springer Verlag, New York, 1985)*.

O. Fackler, M. Mugge, H. Sticker, R. Woerner, and N. W. Winter, "The Calculation of Molecular Final States and Their Effect on a Precision Neutrino Mass Experiment", XIXth Recontre de Moriond, New Particle Production at High Energies (La Plagne, France, March 1984), *Proceedings of Recontre de Moriond (La Plagne, France 1984)*.

#### Abstracts:

John E. Reaugh, James A. Viecelli, and Nicholas W. Winter, "Computer Simulations to study the hot-spot initiation of HMX", *Fall Meeting of the Materials Reseach Society, Boston, MA*, (2003).

Nicholas W. Winter and Francis H. Ree, "Phase stability of small carbon clusters", *Meeting of the American Physical Society, Kansas City, MO*, (1997).

Parkin, S, Marsch, G, Hope, H, Winter, N, Felton, J, "Comparison of crystal structure and theory for 2-amino-1-methyl-6-phenylimidazo[4,5-b]pyridine (PhIP)", *87th Annual Meeting of the American Association for Cancer Research, Washington, DC*, (1996).

Nicholas W. Winter, Mark G. Knize, Mary Tanga, and James Felton, "Structure-Activity Relationships for the TMIP Isomers", *6th International Conference on Carcinogenic and Mutagenic N-Substituted Aryl Compounds*, (1995).

M. A. Lee, N. W. Winter, and James Felton, "Electronic Structure of the 2-Amino-1(3)-Methyl-6-Phenyl-Imidazo[4,5-b] Pyridine Isomers", *6th International Conference on Carcinogenic and Mutagenic N-Substituted Aryl Compounds*, (1995).

T. B. Stewart and N. W. Winter, "Molecular Orbital Calculations of Solid Lubricants", *Annual Meeting of the American Chemical Society, Denver, CO*, (1993).

T. B. Stewart and N. W. Winter, "Molecular Orbital Calculations of the Electronic Structure of MoS<sub>2</sub>", *Annual Meeting of the American Chemical Society, San Francisco, CA*, (1992).

R. M. Pitzer and N. W. Winter, "Spin-Orbit(Core) and Core Potential Integrals", *Workshop on the Methodology of the Evaluation of Integrals in LCAO Calculations*, (1990).

C. E. Violet, R. G. Borg, P. A. Hahn, N. W. Winter, and Z. Mei, "Local Oxygen Configurations Relative to Fe-Probe Ions in HoBa<sub>2</sub>(Cu<sub>0.95</sub>Fe<sub>0.05</sub>)<sub>3</sub>O<sub>7-x</sub>", *International Conference on Materials and Mechanisms of Superconductivity and High Temperature Superconductors*, (1989).

### **Presentations:**

#### Invited Talks:

"Heterocyclic Amines and Their Intermediates Binding to DNA and other Restrained Environments", 42nd Annual Meeting of the Biophysical Society, February 1998.

"Theoretical Evidence for an Optical Gap Closure in Solid N<sub>2</sub>", March Meeting of the American Physical Society, Anaheim, CA, March 1990.

"Experiences in Converting Integral Generation Codes to Operate on Parallel Processors", West Coast Theoretical Chemistry Conference, March 1990.

"The Spectroscopy of High Temperature Superconductors", 44th Symposium on Molecular Spectroscopy, June 1989.

"Theoretical Studies of the Effects of Pressure on the Electronic Transitions in Ruby", Gordan Conference on Research at High Pressure, June 1988.

"Selected Properties of B<sub>x</sub>(x<75) in Ab Initio Model Approximations", American Conference on Theoretical Chemistry, July 1987.

"Theoretical Studies of the Optical Properties of Transition Metal Ions in Crystals", American Conference on Theoretical Chemistry, July 1987.

"Theoretical Studies of Divalent Vanadium in a Magnesium Fluoride Host", Molecular Spectroscopy Symposium, June 1987.